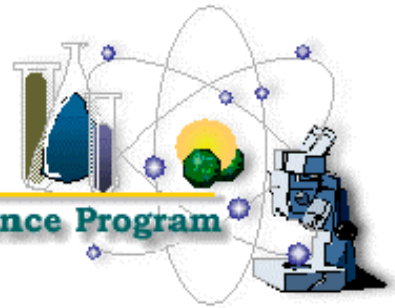
EMSP

Environmental Management Science Program



Modeling of Diffusion of Plutonium in Other Metals and of Gaseous Species in Plutonium-Based Systems

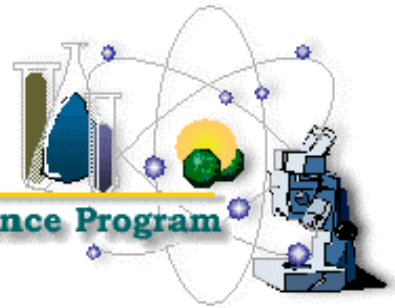
Bernard R. Cooper

West Virginia University

Project No.: 59925
Year of Award: 1997
Project Funding: $435,000

EMSP

Environmental Management Science Program



Project Goals

- To predict diffusion constants on an ab initio basis, i.e. diffusion distances in specified time at specified temperature for plutonium from plutonium-based waste materials into various steels or technologically-pertinent metallic alloys.
  - This predictive ability will help to provide information relevant to setting temperature standards for maintaining structures, ducts, equipment or waste-containing vessels until such time as decontamination and decommissioning and/or permanent storage can be carried out. In addition, this knowledge will aid in assessing the depth of penetration that must be dealt with in any surface treatment for decontamination

EMSP

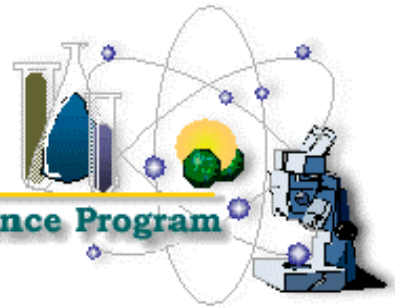
Environmental Management Science Program

Technical Approach

- To recognize the stabilizing mechanism and the electronic structure pertinent to that stabilization for face-centered-cubic (fcc) delta-stabilized plutonium,
- To extract the information needed to perform dynamic simulations from ab initio electronic structure calculations,
- To perform and report the dynamic simulations predicting the diffusion behavior.

EMSP

Environmental Management Science Program

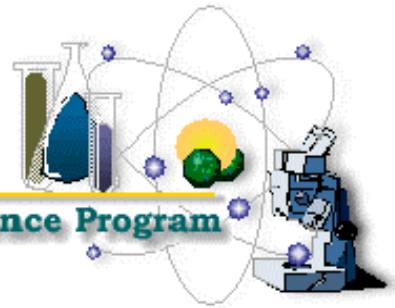


Advantages of Proposed Technology

- The quality of information on the physical and chemical nature and distribution of the plutonium to be provided by the immediate computational modeling predictions and by the proposed portable in-situ characterization apparatus will make this process faster, less expensive, more reliable, and safer

EMSP

Environmental Management Science Program

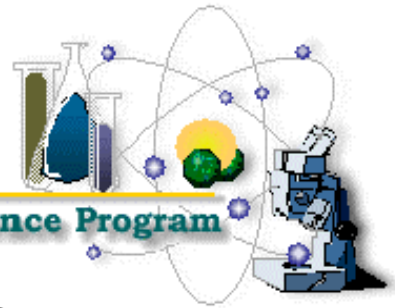


Research End Uses

- Help in designing D&D efforts by predicting the effects of temperature and time on the location of plutonium in steel (or other structural material) building, equipment, or storage components.
- To "look through" steel using x-ray absorption spectroscopy to obtain detailed information about the detailed chemical and physical state of plutonium-contaminated material at sites such as Savannah River, Hanford, and Rocky Flats

EMSP

Environmental Management Science Program



Project Status

- The stabilizing mechanism and the electronic structure pertinent to that stabilization for face-centered-cubic (fcc) delta-stabilized plutonium determined (published May,1999).
  - delta-stabilization occurs through a phase transition to a solid-solution-like phase involving a disordered mixture of two types of plutonium sites (para and ortho plutonium) having the same lattice symmetry but differing 5*f* electronic behavior.
- Extracted information from ab initio electronic structure calculations and perform dynamic simulations to predict diffusion behavior for *3d* transition alloys
  - use to develop the necessary methodology and to provide benchmark results for predictability of experimental behavior..

EMSP

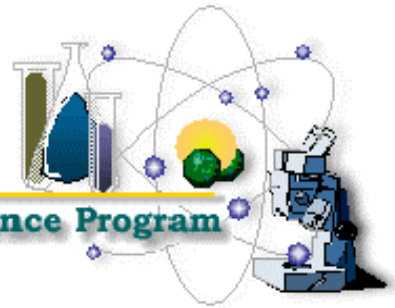
Environmental Management Science Program

Project Status (cont'd)

- Developed technical plan to extract information from ab initio electronic structure calculations and perform dynamic simulations for delta-stabilized plutonium in intimate contact with steel or other structural alloys.
- Plan to demonstrate predictive characterization capabilities of this computational modeling research in conjunction with experiments at LANL for materials containing plutonium.
- Plan to upgrade and employ our rotating anode x-ray source. This will have sufficient x-ray intensity in the relevant spectral range to penetrate steel of the thickness used in ducts, building components, equipment, and containers.
- Need an industrial partner to join in presenting DOE EM with a proposal/plan that will
  - develop the portable XANES (x-ray absorption near edge spectroscopy) apparatus,
  - demonstrate its utility at one of the sites,
  - make clear a plan for its use in the practical on-site D&D work.

EMSP

Environmental Management Science Program



Project Relevancy

STCG Number	Title
RF-DD10S	Decontamination Of Non-Porous Surface